Minutes for the
Basic Energy Sciences Advisory Committee (BESAC) Meeting
February 26-27, 2009
Hilton Washington DC North/Gaithersburg
Bethesda, Maryland

BESAC members present:

Simon Bare
Nora Berrah
Sylvia Ceyer
Peter Cummings
Sue Clark
George Flynn
Bruce Gates
Laura Greene
John Hemminger, Chairman
Bruce Kay
Kate Kirby
William McCurdy, Jr.
Martin Moskovits
Kathryn Nagy
Kathleen Taylor
Douglas Tobias
John Tranquada

BESAC members absent:

Frank DiSalvo
Mostafa El-Sayed
Sharon Hemmes-Schiffer
Michael Hochella
Daniel Morse
John Richards
John Spence

Also participating:

Michelle Buchanan, Oak Ridge National Laboratory
George Crabtree, Argonne National Laboratory
Patricia (Pat) M. Dehmer, Deputy Director of Science Programs, Office of Science
Don DePaolo, Lawrence Berkley National Laboratory/UCB
Wolfgang Eberhardt, BESSY-Berlin
Murray Gibson, Argonne National Laboratory
Jim Horowitz, Basic Energy Sciences
Alan Hurd, Los Alamos National laboratory
Wayne Hendrickson, Columbia University
Franz Himpsel, University of Wisconsin-Madison
Marc Kastner, Massachusetts Institute of Technology
Michael Klein, University of Pennsylvania
Harriet Kung, Director, Office of Basic Energy Sciences
Ray Johnson, BESAC Technical Writer/Recording Secretary
Pat Looney, Brookhaven National Laboratory
Pedro Montano, Office of Basic Energy Sciences
Michael Norman, Argonne National Laboratory
Rick Osgood, Columbia University

Eric Rohlfing, Basic Energy Sciences
John Sarrao, Los Alamos National Laboratory
Rachel Smith, Oak Ridge Institute of Science and Educations (ORISE)
Karen Talamini, Office of Basic Energy Sciences
Katie Perine, Office of Basic Energy Sciences

Approximately 135 others were in attendance in the course of the two-day meeting.

Thursday, February 26, 2009

BESAC Chair **John Hemminger** called the meeting to order at 8:47 a.m. and introduced **Rachel Smith,** who made administrative, safety and convenience announcements. Afterwards, he thanked each member and Sub-Committee for attending.

Hemminger said this BESAC meeting would be unlike others because it would be the first as part of President Barack Obama's administration and the release of the first part of his budget.

He asked **Patricia Dehmer** to update the Committee on the activities of the Office of Basic Energy Sciences (BES). She began her presentation by providing an outline of her presentation, which would include President Obama's plans for science, energy and the environment; Energy Secretary Steven Chu's plans for the Department of Energy (DOE); Budgets, which has hardly been a tidy, linear process this year; factors affecting the economic recession, volatile energy prices and the increased sense of urgency about climate change as a global issue.

In discussing the administration's energy plan, **Dehmer** said that within 10 years, we need to save more oil (than we currently import from the Middle East and Venezuela combined), put one million plug-in hybrid cars – cars that can get up to 150 miles per gallon – on the road by 2015, generate 10 percent of our electricity from renewable sources by 2012 and 25 percent by 2025; and implement an economy-wide, cap-and-trade program to reduce greenhouse gas emissions 80% by 2050.

Next, **Dehmer** discussed the top five priorities and goals. The first priority is in regard to science and discovery. We need to invest in science to achieve transformational discoveries by organizing and focusing on breakthrough transformational science.

She said we need to focus on basic and applied sciences and hopefully double the Office of Science budget. We need to develop and nurture engineering/science talent and support the young, "next generation" of scientists. She said it is imperative that we support these developments in the world and build research networks across department, across the government and globally.

The second priority is to change the landscape of energy demand and supply. We need to drive energy efficiency to decrease energy use in homes, industry and transportation, develop and deploy clean, safe, low carbon energy supplies and enhance DOE's application areas through collaboration with its strengths in Science.

The third priority is economic prosperity. This will mean creating millions of green jobs and increase competitiveness. We would need to reduce energy demand; deploy cost-effective low-carbon clean energy technologies at scale; promote the development of an efficient, "smart" electricity transmission and distribution network; enable responsible domestic production of oil and natural gas and create a green workforce.

The fourth priority is the national security and legacy. We must maintain nuclear deterrent and prevent proliferation; strengthen non-proliferation and arms control activities; ensuring that the U.S. weapons stockpile remains safe, secure, and reliable without nuclear testing and completing legacy environmental clean-up.

The fifth priority is climate change. We must position the United States (U.S.) to lead on climate change policy, technology and science by providing science and technology inputs needed for global climate negotiations; developing and deploying technology solutions domestically and globally and advancing climate science to better understand the human impact on the global environment.

Next, **Dehmer** began discussing the Office of Science FY 2009 (FY09) conference. Virtually all of the FY09 out-year projections are trending upward. BES had a FY08 enacted appropriation of $1,283,402B and the current FY 2008 appropriation is 1,252,756B.

For FY09, the request to Congress is $1,568,160B; the House mark is 1,599,660B; the Senate mark $1,415,378B and the Conference is $1,571,972B. The total Science appropriations are as follows: FY08 enacted appropriation is $4,035,642B; current FY08 appropriation is 4,082,883B. For FY09, the request to Congress is $4,721,969B; the House mark is 4,861,669B; the Senate mark $4,640,469B and the Conference is $4,772,636B.

The Office of Science FY08 budget, appropriations and supplemental are as follows:

	FY 2008		
	Prior Approp.	Supple-mental	Current Approp.
Basic Energy Sciences	1,269,902	+13,500	1,283,402
Advanced Scientific Computing	351,173	—	351,173
Biological and Environmental Research	544,397	—	544,397
High Energy Physics	689,331	+32,000	721,331
Nuclear Physics	432,726	+1,500	434,226
Fusion Energy Sciences	286,548	+15,500	302,048
Science Lab Infrastructure	66,861	—	66,861
Science Program Direction	177,779	—	177,779
Workforce Development	8,044	—	8,044
Safeguards and Security	75,946	—	75,946
Subtotal, Science	3,902,707	+62,500	3,965,207
ARPA-E	—	—	—
Safeguards and Security (reimbursable charge)	-5,605	—	-5,605
Congressionally-directed projects	123,623	—	123,623
Rainforest Rescission	-44,569	—	-44,569
Use of prior year balances	-3,014	—	-3,014
Undistributed	—	—	—
Total, Science	3,973,142	+62,500	4,035,642

Dehmer then looked at a 12-year history of requests versus appropriations for SC programs. Over the past few years, all programs fell short, with the only program seeing an increase was Appropriations for Advanced Scientific Computing Research (ASCR).

The economic stimulus package is formally known as ARRA. The FY09 recovery act appropriation for all sciences is $1.6B.

The House Representative 1 - the American Recovery and Reinvestment Act of 2009 - For spending, The House bill introduced on January 26 was $550B, plus $275B tax cuts ($825B total cost). The Congressional Budget Office (CBO) analysis of original House bill is $604B, in addition to $212B for tax cuts ($816B cost). The CBO analysis of House-approved bill is $637B, plus $182B for tax cuts ($819B).

Democrats say tax cuts represent one-third of the overall stimulus package, not a huge difference from President Obama's original goal of 40 percent. But, congressional budget analysts count nearly $100 billion of these measures as spending because they are credits are going to people who don't pay taxes. The CBO adjustment reduces the tax-cut portion of the package to 22 percent.

The CBO divides the bill's spending into direct payments to individuals (i.e. unemployment compensation or tax credits) and purchases of goods and services, either directly by the federal government or indirectly in the form of grants to states and local governments. "There is incredible pressure to use the money well and wisely," said **Dehmer**.

A charted breakdown of the House Plan outlays from 2009 through 2019 was shown, with Energy and Water getting $48.9B. Within this amount, $18.5B will go to energy efficiency and renewable energy programs, $8B for Federal loan guarantees for renewable-energy systems and electricity transmissions, $17.4B for others, including modernizing the nation's electricity grids and $4.5B for Army Corps of Engineers. Health, labor and education ($91.3B), Medicaid ($89.7B) and Tax Provisions ($82.1B) received the largest outlays.

With the 2009 Supplemental Recovery Funding for research and development (R&D), including House, Senate and Final bills for DOE Science, the House has approved $1.6B; the Senate $.33B and Final bills $1.6B.

The ARRA categories of support in SC are:

- Facility Construction – Funds accelerate completion of a number of ongoing construction projects for major scientific user facilities, major items of equipment for those facilities and laboratory infrastructure. General Plant Projects (GPP) update laboratory infrastructure and establish new laboratory research space, renovate existing laboratory space, demolish inadequate facilities and improve utility systems across SC labs.
- Facility Operations/Infrastructure – Funds increase operations, experimental support and infrastructure improvements at scientific user facilities across SC
- Research – Funds support selected research programs across SC and are chosen to minimize out-year mortgages. Energy Frontier Research Centers are included.
- Computing – Funds support advanced networking; mid-range distributed computing; and computation partnerships in areas important to DOE energy missions.

- Fellowships – A program to support graduate students and early career scientists was proposed by SC and is under discussion within DOE

The "Next Generation Photon Sources for Grand Challenges in Science and Energy" is a report of a subcommittee to the BES Advisory Committee. **Dehmer** looked at the energy sources and consumption sectors in the U.S. The U.S. Energy Flow in 2007 showed that approximately 33 percent of the U.S. primary energy is imported. With energy supply in quads, domestic productions accounted for 71.7 quads, imports had 34.6 quads and exports 5.4 quads, equaling 101.6 quads in energy consumption.

The next few charts **Dehmer** discussed included three classic energy flow diagrams showing energy supply and energy consumption. Eighty-five percent of primary energy is from fossil fuels, with 67% domestic and 33% imports. The U.S. Energy Flow of 2006 showed greater than 70 percent of primary energy for the transportation sector and more than 60 percent of primary energy for electricity generation/use is lost.

Key R&D strategies and how basic science will influence technology. Electric energy storage, electricity distribution, end-user efficiency, conservation, climate/environment impacts, fuel switching are all instrumental.

Dehmer concluded her presentation by saying the current budget is waiting on Senate approval. "We look forward to some exciting times in the coming months."

Hemminger asked the Committee and Sub-Committee members if they had any question for **Dehmer**.

Marc Kastner said he agrees with **Dehmer** that "this is a wonderful time."

Bruce Gates asked what degree of climate change is affecting DOE.

Dehmer said the Office of Science is looking at atmospheric modeling and climate change.

Kate Kirby said this "looks good for students." She asked if the funding will be distributed quickly for graduate students.

Dehmer said "we will have to put some thought into this and it will 'lag behind' other projects in priorities.

Hemminger said he believes details will be coming out very quickly.

At 9:35 a.m., **Hemminger** introduced **Harriet Kung** to provide news from the Office of Science (SC).

Kung provided an outline by providing an outline of her presentation, which will include an update on the new administration and DOR, BES budget and staffing updates, EFRC/SISGR status, BES and photo science and lastly and NAS catalysis program review.

Kung said that Dr. Steven Chu was named the Office of the Secretary under President Obama. There are several vacancies currently including the Deputy Secretary (reporting to Chu); Office of the Under Secretary; and the Office of the Under Secretary for Science.

Kung said that there had been several statements made over the past six weeks that she would like to share regarding the investment in science to achieve transformational discoveries. President Obama said in his Inaugural Address: *"We will harness the sun and the winds and the soil to fuel our cars and run our factories."* In President Obama's discussion concerning energy at the joint session of Congress (February 24, 2009), he said it is "absolutely critical to our future," "it is time for America to lead again," "To truly transform our economy, protect our security, and save our planet from the ravages of climate change, we need to ultimately make clean, renewable energy the profitable kind of energy, … And to support that innovation, we will invest fifteen billion dollars a year to develop technologies like wind power and solar power; advanced biofuels, clean coal, and more fuel-efficient cars and trucks built right here in America." and "the answers to our problems don't lie beyond our reach. They exist in our laboratories and our universities." Secretary Chu said "As a scientist, I understand the seriousness of the economic and climate challenges we face. But I remain optimistic that scientific research will once again bring us transformative solutions."

Kung said she would continue where **Pat Dehmer** left off in stating The American Recovery and Reinvestment Act of 2009 was passed by Congress February 12 and signed by President Obama February 17. The Act includes $288B for Tax Relief; $144B for State and Local Fiscal Relief; $111B for Infrastructure and Science; $81B for Protecting the Vulnerable; $59B for Health Care; $53B for Education and Training; $43B for Energy and $8B for others.

BES plans to invest the additional funding received from the American Recovery and Reinvestment Act of 2009 in the following areas: 1) accelerate constructions projects and major items of equipment completion 2) Implement capital equipment augmentation 3) Support priority research.

Next, **Kung** reviewed the Office of Science FY 2009 Budget Request. For BES, $1,221,380B was appropriated in FY07 and $1,269,902B was appropriated in FY08. For FY09, the request sent to Congress is $1,568,160B, which is $298,258M (+23.5%) more than the FY08 appropriation. For the Office of Science, the FY09 Request to Congress is $4,721,969B, which is $748,827M (+18.8%) more than the FY08 appropriation.

For the FY09 Energy and Water Development Appropriations for BES, **Kung** discussed the House and Senate Reports. The House Report states, "The Committee recommendation for BES is $1,599,660B, an increase of $31.5M over the budget request and an increase of $329,758M over the current fiscal year. For purposes of reprogramming during fiscal year 2009, the Department may allocate funding among all operating accounts within BES, consistent with the reprogramming guidelines outlined earlier in this report." The Senate report said "The Committee provides $1,415,378B for BES. Of these funds $145,468M is provided for construction activities as requested in the budget. The remaining $1,269,910B is for research. Within the research funds provided $17M is for the Experimental Program to Stimulate Competitive Research [EPSCoR]. Of the decrease, $59,495M of basic solar research is moved to the EERE solar energy research and development program."

Next, **Kung** discussed the H.R.1105 - Omnibus Appropriations Act, 2009 and the Energy and Water Development and Related Agencies Appropriations Act, 2009. For BES, the bill provides $1,571,972,407 for this program. Within this amount, $17M is provided for the EPSCoR. Full funding is provided to support the operations of the major scientific user facilities and the five Nanoscale Science Research Centers, as well as additional instrumentation for the Spallation Neutron Source and the LINAC Coherent Light Source. The control level is at the BES level.

One of the top priorities for the BES program is to invest in science to achieve transformational discoveries. Kung said we must expand the core research program, such as having large-scale research centers and collaborations (such as the EFRCs); single investigator and small group research; broader EPSCoR participation; support world-class scientific user facilities, such as synchrotron light sources; neutron scattering facilities; electron micro-characterization facilities; Nanoscale Science Research Centers; and new construction and instrumentation, such as National Synchrotron Light Source-II, LINAC Coherent Light Source + LINAC operations + instruments; Advanced Light Source User Support Building; Spallation Neutron Source instruments; and PULSE Building.

Regarding the FY10 budget, **Kung** stated on February 26, the Administration's FY10 Budget Overview will be released. The agency summaries in the overview provide highlights of the agency budget. The overview also describes certain administration initiatives and other proposals. DOE will not make commitments about specific programs not specifically mentioned in the overview or address account level details until the release of the full budget in April.

Kung offered a look at the Office of BES. She said there were many openings in the different divisions and actively looking to fill these positions and requested BESAC members assist in finding suitable candidates. Some of the recent hires have been Committee Manager **Katie Perine,** Program Analyst/BESAC and **Ehsan Khan**, Program Manager in the Materials Sciences and Engineering Division, reporting to **Jim Horwitz**.

Next, **Kung** provided an update on Energy Frontier Research Center (EFRC) and Single-Investigator and Small-Group Research (SISGR). She discussed the December 2008 report, *New Science for a Secure and Sustainable Energy Future Report.* She said the report is "serving the present and shaping the future." The present pace of change for clean energy technologies is not sufficient to meet future needs. BES must lead a major campaign focused on increasing the rate of discoveries and establishing U.S. leadership in next-generation carbon-free energy technologies. She also stated that significant discoveries will come at the intersection of control science with complex functional materials. BES must move aggressively in these directions lest the U.S. fall behind in the global competition for the discoveries that underpin future energy sources, systems and processes. **Kung** said it will take "dream teams" of highly-educated talent, equipped with forefront tools and focused on the most pressing challenges to increase the rate of discovery. To make progress most rapidly, these teams must work to close gaps between needs and capabilities in synthesis, measurement, theory and computation. U.S. leadership requires BES to lead a national effort to aggressively recruit the best talent through a series of workforce development aimed at inspiring today's students and young researchers to be the discoverers, inventors and innovators of tomorrow's energy.

The EFRC is tackling energy challenges in a new era of science and engaging the talents of the nation's researchers for the Broad Energy Sciences. BES announced the initiation of EFRCs to accelerate the scientific breakthroughs needed to create advanced energy technologies for the 21st century. The EFRCs will pursue the fundamental understanding necessary to meet the global need for abundant, clean and economical energy.

EFRC will pursue collaborative fundamental research that addresses both energy challenges and science's grand challenges in areas such as:

- Solar energy utilization
- Catalysis for energy
- Electrical energy storage
- Solid state lighting

- Superconductivity
- Geosciences for nuclear waste and CO_2 storage
- Advanced nuclear energy systems
- Combustion of 21st century transportation fuels
- Hydrogen production, storage and use
- Materials under extreme environments
- Conversion of biological feedstock to portable fuels
- Others

The timeline for the EFRC solicitation is as follows: In February 2008, BES rolled out EFRC in FY09 budget request and BESAC; in April 2008, EFRC FOA issued amended (also in 4/2008, 6/2008 and 9/2008); in April 208, BES received 251 letters in intents; in October 2008, BES conducted interviews; in April 2009, awards will be announced, pending appropriations.

The EFRC merit review evaluation, as described in the EFRC FOA, Part V, Application Review Application includes:

Initial Review (DOE):

- For eligibility of the applicants and institutions, per the criteria set forth in the FOA Part III, Eligibility Information
- For completeness of the application
- For responsiveness to the objectives of the FOA, particularly addressing both a science grand challenge and one or more energy research challenge
- Applications failing the initial review will be declined without further merit review; applicants will be notified and provided with the declination justification

Merit Review (External Scientific Experts):

- Applications will be evaluated by one or more Merit Review Panels (MRPs)
- The breadth of science encompassed by the FOA will require multiple MRPs
- Each application will be reviewed using these four criteria, with additional sub-criteria described in detail in the FOA:
    - Scientific and/or technical merit of the project
    - Appropriateness of the proposed method or approach
    - Competency of the applicant's personnel and adequacy of the proposed resources
    - Reasonableness and appropriateness of the proposed budget
- Following the merit review, a team of federal officials will review the applications and the evaluations of the MRPs, summarize the MRP's independent evaluations and recommend the application of other selection factors to the selection official.

Award Selection (DOE):

- Other selection factors: diversity of research activities, relation of the proposed EFRC to the ongoing programs in BES, potential for developing synergies between the proposed EFRC and other EFRCs or ongoing BES research and the total amount of DOE funds available
- The selection official will consider the evaluations of the MRPs, federal official's recommendations and other selection factors in making award decisions

With SISGR, **Kung** discussed tackling energy challenges in a new era of science. SISGR will significantly enhance the core research programs in BES and pursue the fundamental understanding necessary to meet the global need for abundant, clean and economical energy. Awards are planned for three years, with funding in the range of $150-300K per year for single-investigator awards and $500-1,500K per year for small-group awards. The areas of interest include: **Grand challenge science**: ultrafast science; chemical imaging, complex and emergent behavior; **Use-inspired discovery science**: basic research for electrical energy storage; advanced nuclear energy systems; solar energy utilization; hydrogen production, storage, and use; geological CO_2 sequestration; other basic research areas identified in BESAC and BES workshop reports with an emphasis on Nanoscale phenomena; and **Tools for grand challenge science*:*** mid-scale instrumentation; accelerator and detector research (exclude capital equipment supports).

The SISGR solicitations had 879 whitepapers, with 88% from universities, 11% from DOE labs and 1% from other institutions. Energy sources (i.e. advanced nuclear energy system, solar energy utilization and geological sequestration of carbon dioxide) accounted for 31% of the papers; Grand Science Challenges and Tools (ultrafast science, chemical imaging, mid-scale instrumentation and complex systems and emergent behavior) accounted for 28%. In addition, energy storage (16%), cross-cutting (15%) and energy efficiency (10%) were included.

The timeline of the SISGR began in February 2008, with BES discussing the SISGR plan at BESAC. In April 2008, BES issued a SISGR Web notice. By October 2008, BES received approximately 880 whitepapers. By March 2009, it is tentatively scheduled that BES will notify PIs of whitepaper decisions. In April 2009, full proposals are tentatively due to BES. In June 2009, BES is tentatively scheduled to issue SISGR awards.

Next, **Kung** discussed the BESAC Workshop on Solving Science and Energy Grand Challenges with Next Generation Photon Sources. The photon workshop was held October 27-28, 2008, with **Wolfgang Eberhardt** and **Franz Himpsel** serving as Co-Chairs. The workshop charge included:

- Identify connections between major new research opportunities and the capabilities of the next generation of light sources ("photon attributes," such as coherence and femtosecond time resolution). There will be particular emphasis on energy-related research. The presentations and discussion sessions will highlight how time-resolved excitation, functional imaging, diffraction and spectroscopy by photons can help solving major problems and develop "killer applications" in BES. A variety of opportunities have been outlined by 10 BESAC and BES reports on basic research needs and by a report on five "Grand Challenges" in directing matter and energy.
- Both accelerator-based light sources and novel laser-based sources for the VUV to X-ray range will be considered. The photon workshop will identify the science drivers for new photon sources, but will not consider the design of machines or devices for producing the required photons. A strong coupling of theory and experiment will be emphasized.
- A matrix will be prepared to define the most compelling connections between research opportunities and photon attributes. For example, many science and energy grand challenges require probing very fast processes that happen over very small distances: femtoseconds over nanometers. Typically, an electron in a solid takes a femtosecond to travel a nanometer, and atoms have a vibrational period of about 100 femtoseconds. Lasers probe femtoseconds and synchrotrons resolve nanometers, but presently neither can do both.
- The photon attributes to be considered by the workshop include coherence length (longitudinal and transverse), time structure, energy, energy resolution, spectral brightness (average and peak), flux, spatial and momentum resolution and polarization.

The four BES light sources hosted 8,492 users in FY08 – APS (39%), NSLS (25%), ALS (23%) and SSRL (13%). The size and demographics of the user community have changed dramatically since the 1980s when only a few hundred intrepid users visited the synchrotron light sources each year. With the discussed graph, **Kung** said now the "user" is a researcher who proposes and conducts peer-reviewed experiments at a scientific facility or conducts experiments at the facility remotely. A user does not include individuals who only send samples to be analyzed and pay to have services performed or visit the facility for tours or educational purposes. Users do not include researchers who collaborate on the proposal or subsequent research papers, but do not conduct experiments at the facility. For annual totals, an individual is counted as one user at a particular facility no matter how often or how long the researcher conducts experiments at the facility during the year. The characteristics of the users and the nature of the research were 97% for nonproprietary research only, 31% were first-time users and 27% were female.

Constrained budget appropriations have hindered the growth in the number of users. **Kung** said the BES programs provide complete support for the operations of the facilities. Furthermore, BES continues as the dominant supporter of research in the physical sciences, providing as much as 85% of all federal funds for beam lines, instruments and PI support. Many other agencies, industries and private sponsors provide support for instrumentation and research in specialized areas such as protein crystallography.

For the four BES light sources, the majority of users continue to be from academia. The number of users from the host institutions has grown from the early days, reflecting a commitment on the part of the host institutions to these user facilities. Notably, the fraction of industrial users has declined over the past 18 years, reflecting the trend of industry to move away from fundamental research.

Kung showed a graph showing that California, Illinois and New York account for the most BES light sources. California is host state for SSRL and ALS. Illinois is host state for APS. New York is host state for NSLS.

Kung discussed the National Academy of Science Review of the BES Catalysis Science Program:

- **Sec. 973 of the Energy Policy Act of 2005 (EPAct 2005) states:**

"(d) Assessment – Not later than three years after the date of enactment of this Act, the Secretary shall enter into an arrangement with the National Academy of Sciences to- (1) review the catalysis program to measure – (A) gains made in the fundamental science of catalysis; and (B) progress towards developing new fuels for energy production and material fabrication processes; and (2) submit to Congress a report describing the results of the review."

- **In compliance with EPAct 2005, in 2007 BES requested that the NAS Board on Chemical Sciences and Technology conduct this review to:**
    - Examine the BES research portfolio in catalysis and identify whether and how this portfolio has advanced fundamental science in this area
    - Discuss how the BES research portfolio in catalysis contributes and is likely to contribute to immediate and long-term national energy goals, such as reducing the nation's dependence on foreign sources of energy

- **The NAS committee requested and received a significant amount of information from BES regarding the catalysis science program, including but not limited to:**
    - A complete listing of supported projects (classified by area) and investigators from 1997-2007
    - A description of multi-investigator collaborative projects and how such projects are incentivize
    - The historical context for the program, including mission statements going back more than 20 years
    - The top success stories in the program over the last decade
    - The influence of BES workshops on the program over time
    - The measures taken by BES to ensure continuity of the research enterprise in catalysis science
    - Funding for instrumentation within the program

- **The committee held several meetings to conduct the review and received information through talks and interviews with:**
    - DOE program staff from BES and the technology offices (EERE and FE)
    - Catalysis experts from academia, industry, and DOE laboratories
    - Principle investigators in the BES Catalysis Science Program
    - The co-chairs of the BES workshop: *Basic Research Needs: Catalysis for Energy*

The top BES Catalysis Science stories are:

- BES provided nine "success" stories to the NAS review committee to demonstrate the impact of the BES Catalysis Science Program in the last 10 years. Each story represents a significant body of work supported over time by BES and is based primarily on the work done by the research group of the investigator noted in parentheses.
- Shared the 2005 Nobel Prize in Chemistry with Robert Grubbs and Yves Chauvin for work that led to the understanding of the mechanistic steps of olefin metathesis and the development of successfully working catalysts for such chemistry. Olefin metathesis is a chemical process that is largely responsible for the production of fuels, pharmaceuticals, polymeric materials, detergents, and many other petrochemical products. Through exquisite control, catalysts direct organic molecules that might not react under mild conditions, to link together in specific ways and with minimum production of waste.

Kung concluded her presentation by discussing how the NAS committee summarized the historical and current impacts of the program in two traditional areas: Heterogeneous catalysis – surface science, nanoscale catalysis, and theory; Homogeneous catalysis – single-site polymerization, C-H activation and functionalization, organic synthesis and bio-inspired catalysis. The review provided an endorsement of the BES Catalysis Science Program and useful guidance in areas where the portfolio could be strengthened. As summarized on the NAS web site: "the report concludes that the program has invested well in catalysis basic research. The program's success can be attributed to key management decisions over the past eight years that have led to a current funding distribution that advances catalysis science in general and keeps the development of energy-related technologies as a long-term goal. The program has maintained support for many well-established and world-renowned leaders in catalysis and, at the same time, has brought in many new researchers. The DOE Catalysis Science Initiative has been a particularly effective mechanism for bringing to the program new funds, new researchers, and innovative research topics -- especially in heterogeneous catalysis." The review recommended modest changes in the portfolio that are consistent with BES strategic planning:

- Heterogeneous catalysis – maintain high surface area catalysis, surface science, nanoscience, and electrocatalysis, but put increased emphasis on catalyst design, new synthesis methods, unique reactor systems, unique characterization techniques, and completely new chemical reactions.
- Homogeneous catalysis – portfolio should extend beyond individual mechanistic steps to include greater development of new catalytic systems and reactions. Portfolio improvement suggested in: C-H bond functionalization, new approaches to transition-metal catalysis, and electrochemical catalysis. In addition, a greater emphasis should be placed on reducing highly oxidized compounds, such as bioderived materials into fuels and feedstocks, and on bio-inspired catalytic processes.

At 10:25 a.m., **Hemminger** declared a 30-minute break.

At 10:58 a.m., **Hemminger** called the meeting back to order and requested each Committee and Sub-Committee member introduce themselves and their respective affiliations.

At 11:03 a.m. **Hemminger** introduced **George Crabtree. Hemminger** said the BESAC report, *New Science for a Secure and Sustainable Energy Future Report* that **Crabtree** and **Marc Kastner** served as co-chairs, was approved. **Hemminger** said it was a "very thought provoking report," was nicely done and had substantial implications. He said that we will discuss tomorrow options to getting these reports out as soon as possible.

Crabtree began his presentation buy discussing his presentation would include an outline and background of the project, the photon workshop and report preparation. The New Era Subcommittee of BESAC includes **Crabtree** and **Kastner**, as well as several people in attendance at the meeting. **Michelle**

Buchanan, Thomas Mallouk, John Sarrao, Michael Klein, Arthur Nozik, Julia Phillips, Sue Clark, Frank DiSalvo, Don DePaolo, Simon Bare, Wayne Hendrickson, Wolfgang Eberhardt, Franz Himpsel, Michael Norman, Andrea Cavalleri, Carl Lineberger, Yet-Ming Chiang, Pat Looney were acknowledged for their hard work on the project. In addition, **Roger Klaffky, Michael Casassa, Jim Horwitz** offered technical support.

The background of the project was examined, with Crabtree stating the New Era concept was first discussed with BESAC at the February 21-22, 2008 meeting. The first New Era meeting was held July 24-25, immediately following the summer BESAC meeting. There was a three-part charge:

- Summarize basic research needs and Grand Challenge reports
- Recommend implementation plans to address the challenges
- Identify grand energy and science drivers for future light sources and the "photon attributes" required to pursue them. Parts I and II concern new science reporting, which will be discussed Friday morning. Part III will be discussed this morning, which concerns the photon workshop report.

As mentioned earlier, **Eberhardt** and **Himpsel** served as co-chairs for the Photon Workshop October 27-28. The guidelines were to solicit broad community input, focus on science drivers and photon attributes required to pursue them, no consideration of specific machine designs, survey photon attributes of existing and envisioned classes of photon sources: third generation storage rings, energy recovery , free electron lasers, high harmonic generation lasers and lastly, identify "killer applications" that are especially compelling.

Crabtree discussed the program organization of the workshop, with the morning plenary sessions for background, breakout group on nine science areas and plenary reports of the breakout groups. There was also a post-workshop writing day for the breakout chairs. In addition, there was a photon workshop website developed for ongoing communication among participants.

After the workshop was held, the breakout groups refined the content and organized the science drivers into five cross-cutting challenges and three stages of difficulty. There was consultation with recent reports on future light sources from the U.S., Europe and Asia. There were comments on drafts from breakdown chairs and New Era Sub-Committee members. The final revision was received on February 16.

At 11:00 a.m., **Hemminger** requested all comments by the Committee and Sub-Committee be held until later in the afternoon. He promptly introduced **Franz Himpsel** to provide an update concerning the Photon Workshop, *Next Generation Photon Sources for Grand Challenges in Science and Energy.*

Himpsel told the Committee how the report was "split up" and said he would be discussing the "greatest opportunities." He will be covering Sections 1-4 of the report and **Eberhardt** will do the others.

Himpsel began his presentation by discussing the third charge from BESAC to the New Era Committee. The charge stated that we must identify new science and the photon attributes of the next generation light sources required to carry it out, such as: energy range (from vacuum UV to hard X-rays), coherence, time resolution (femtosecond regime), brilliance (average, peak) and polarization (circular, linear).

The charge to the participants of the workshop was to:

- Identify connections between major research opportunities and the capabilities of next generation light sources
- Find "killer applications" that could become scientific drivers
- Emphasize energy-related research and life sciences
- Consider the VUV to X-ray range and include both accelerator-based light sources and laser-based sources
- Do not choose a specific light source design, consider only the photon attributes required for the most promising research
- Strong coupling of theory and experiment

There were approximately 100 participants in the workshop, providing overview talks concerning energy and life sciences; next generation light sources concerning free electron lasers, energy recovery linacs, high harmonic lasers and next generation storage rings. The breakout groups had extensive discussions and highlighted their one and a half day meetings with a write-up.

The breakout groups discussed a variety of subjects, with some of the coordinators being BESAC members (**Hemminger** and **Nora Berrah**). The group generated an extensive number of scientific opportunities, which is detailed in Section Four of the report. Among the subjects are Nanoscale electrons and spins; Correlated electrons; Catalysis and chemistry; Nano-materials for energy applications; Life sciences; Atomic and molecular physics; Matter under extreme environments and environmental science, earth science; Novel structural and electronic materials and the cross-cutting issues.

The findings are five cross-cutting challenges, with three stages of difficulty. The first stage (Stage A) is designing materials, controlling processes and the synthesis-analysis-prediction loop. The second stage (Stage B) is real-time evolution of chemical reactions, movement of electrons and spin, as well as individual nano-objects. The third stage (Stage C) is statistical laws of complex systems, small and fast.

The three stages of difficulty are:

Stage A:
- Widest range of applications, largest user community
- Least aggressive in terms of machine requirements (but clearly beyond available light sources)

Stage B:
- Novel experiments, demanding a new kind of light source
- Widespread applications, many potential users
- Could become the centerpiece of next generation light sources

Stage C:
- Most aggressive, highest risk, highest potential payoff

The "Sweet Spot" is Stage B with the temporal evolution of electrons, spins, atoms and chemical reactions, down to the femtosecond. In addition, the probing isolated nano-objects or nano-regions of unhomogeneous samples, either by spectroscopy with an energy resolution smaller than the intrinsic line width or by imaging with a spatial resolution at the atomic limit. The active Fe_6Mo center of nitrogenase, nature's efficient way of fixing nitrogen is to resolve the chemical reaction steps in time, questions the resulting structural changes and determines the charge flow by spectroscopy.

Himpsel showed a comparison with the NSF study. The science case was probing picoseconds properties of magnetic materials. There are some exciting new scientific frontiers in areas such as lenseless imaging and ultrafast dynamics and spectroscopy are enabled by these properties. Exploiting this scientific frontier in the U.S. is essential for our competiveness in strategic areas of science, engineering, workforce development and could have significant commercial impact.

The following is from The Berkeley Workshop Report and addressed the scientific areas by new light sources Chemical Physics; Atomic, Molecular and Optical Physics; Magnetization and Spin Dynamics; Correlated Materials; and Exploration of Nanoscale Dynamics and Complexity. **Himpsel** said "light source under construction or on the drawing board can deliver the beams required for the cutting edge science described in this document."

The White Paper report was prepared by scientists from Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), Lawrence Berkeley National Laboratory (LBNL) and SLAC National Accelerator Laboratory, including the University of California and Stanford University. The collaboration consisted of scientists from a broad range of scientific disciplines and included experts in x-ray and accelerator science, two core competencies of these four laboratories. The four labs play a key role in the DOE Complex of National Laboratories, operating forefront X-ray programs on the second-generation storage ring NSLS, the third-generation storage rings ALS, APS and SPEAR-3 and have forefront knowledge of advanced sources based on the construction of LCLS, the first hard X-ray laser, to be commissioned in 2009, and NSLS-II, an advanced third-generation storage ring to be commissioned in 2013. Information was also provided and coordinated with external experts and colleagues from around the world.

The scientific drivers include the following:

1) *atomic and molecular science*—studying fundamental processes involving atoms, electrons and spins;
2) *chemical reactivity*—discovering the key far-from-equilibrium processes related to energy production, climate change, and environmental processes;
3) *complex materials*—a core subject of condensed-matter physics and engineering sciences, which often drive technological advances—and their materials synthesis;
4) *materials under extreme conditions*—revealing new synthesis pathways of tailored matter and discovering the limits of materials stability, performance, and function;
5) *life sciences and soft matter*—studying the structure and dynamics of organic building blocks of technological materials promising the improvement of health.

Himpsel provided examples for possibilities: The *Basic Research Needs for Solar Energy Utilization* and *Basic Research Needs: Catalysis for Energy*. These workshops from 2005 and 2007 respectively show how organic molecules with a transition metal as the active center (LEDs, solar cells, enzymes equal bio-catalysts) detect oxidation state, spin state ligand field for one Fe atom.

Himpsel questioned what happens during a photochemical reaction. These measurements on the 100 picoseconds time scale provide information about spin excitations and their lifetime. To learn about structural dynamics one needs 100 femtosecond (fs) time resolution, and for electronic excitations a few fs. That is only possible with next generation light sources.

In spatially resolved catalytic reactions, we want this chemically resolved, but you will have insufficient spatial resolution. He also showed the Fischer-Tropsch process for converting coal to liquid fuel.

In fast switching of spins, low power electronics, switching of spins requires little energy, but questions if it can be fast. The limit is given by uncertainty relation. **Himpsel** questioned how the angular momentum gets absorbed in a surprisingly fast switching of spins in the femtosecond range.

Proteins in action can observe slow recombination, but not yet the fast initial biochemical reaction. Time-evolution of a protein structure after stimulating the

Fe atom in the heme controls materials atom by atom. The energy gap between the highest occupied and lowest unoccupied energy level of mass-selected atomic clusters was also examined. We need higher photon energy to see all the other energy levels.

Towards Spectroscopy of an Isolated Nano-Object, we need to reach atomic precision in nanotechnology. Optical spectra of self-assembled quantum dots show a broad continuum due to the size distribution. Selecting fewer dots with smaller apertures reveals the discrete line spectrum expected from an isolated dot ("artificial atom"). We need higher photon energy to access all levels, including core levels.

In conclusion, **Himpsel** said there are two science drivers ("killer-apps") for new light sources are identified which combine the deepest science impact with the broadest user base:

- Femtosecond time resolution opens completely new territory where atoms can be followed in real time and electronic excitations can be resolved down to their intrinsic time scale
- Sub-nanometer spatial resolution opens the length scale where quantum confinement dominates electronic behavior and where catalytic activity begins. Spectroscopy of individual nanometer-scale objects, rather than conglomerates, will eliminate blurring of the energy levels induced by the size and shape distribution and thereby reveal active sites in catalysis and the traps where electrons are lost in photovoltaic.

Hemminger said he would like to request **Wolfgang Eberhardt** begin his presentation after lunch. The meeting was adjourned at 11:58 p.m.

At 1:37 p.m., **Hemminger** introduced **Eberhardt** to continue the discussion regarding the report of the Sub-Committee to the BES Advisory Committee. **Eberhardt** said storage rings are the foundation of success of synchrotron radiation research. The insertion devices are the sources of high brilliance radiation. Brilliance: Photons/$mm^2 mrad^2$ s DE I; Emittance: e (nmrad); With the Wiggler: Intensity ~ n, Continuous spectrum, higher photon energy; with Undalator, Brilliance ~ n^2, discrete harmonics and one e^- coherence.

The storage rings have the following characteristics:

Photon Parameters

- Energy Range Thz to > 100 keV
- Energy resolution E/DE 10^4 to $>10^6$
- Independently tuneable
- Selecteable polarization

- Pulse length 30 ps
- Partially coherent
- Many (50) simultaneous experiments

Electron Parameters

- 1.5 GeV < E < 8 GeV
- energy spread > 0.1%
- bunch charge 1nC
- 500 MHz rep-rate
- Total current 300 mA
- ~ E^2/R typically (1-10 nmrad)

Next, **Eberhardt** looked at the average brillance versus the amount of photon energy and the influence of the electron beam emittance. He also questioned how can we improve X-ray sources.

Self Amplified Spontaneous Emission operation shows that all electrons emit coherently, with a brillance proptional to $n_{el}^{2.}$ It has en extremely high peak brillance, fully coherent team and fs pulses. The peak brillance in the X-ray range is unmatched by any other source.

The temporal pulse shape of the FLASH FEL is measured by autocorrelation. **Eberhardt** said showed the visability of the interference fringes (visibility versus delay (fs) and the model of the pulse shape (12 fs pulses are realizable).

In photon sources and FEL's, all ectrons emit conherently with a brilliance proptional to n_{el}^2. There is an extremely high peak brilliance and a fully conherent beam. The FEL facility operations has:

- High Peak Power --- High Peak Brilliance --- Full Coherence --- fs Pulses
- Seeded FEL's : synchronized pulses with reproducible, controllable shape
- Unusual multi-bunch pattern (5 Hz to 120 Hz with pulse trains)
- Intrinsic energy resolution $E/DE \leq 10^3$
- Few user operation ---- not fully independent
- Not rapidly tuneable (discrete selectable energies)

Energy recovery LINAC combines advantages of storage rings with accelerator driven sources.

- High average brilliance ---- coherence ---- short (1ps) pulses (fs option)
- Many independent experiments ---- UV to hard X-rays --- long (25m) undulators
- Round beam (novel undulator designs)
- Very flexible pulse patterns (multiple injection systems) ---- GHz rep rate

In addition, energy recovery LINAC has high average brilliance, a very flexible operation, multiple injection system parameters, high current --- high coherence and short (50 fs) pulses.

Eberhardt looked at third generation X-ray sources versus fourth generation. Third generation (storage ring) has many experiments, ready tunability, high flux and ps pulses. With fourth generation, LINAC source is has extremely high peak brilliance, full spatial coherence, ultrashort (fs) pulses, temporal coherence with seeding, low pulse rep. Rate 10^2 to 10^5 Hz and few experiments. Also in fourth generation, Energy-Recovery LINAC has high avarage brilliance, full spatial coherence, many experiments, ready tunability, excellent energy resolution, flexible pulse characteristics, Fs to ps pulse lengths and 10^9 pulses/s.

Next, **Eberhardt** discussed the ultimate storage ring and the difference between ERL and FEL.

- Lasing is special to the FEL --- 10^6 more photons/pulse
- FEL's and ERL's can use the similar gun designs (injection system) and the electron beam is determined by the accelerator system
- Diffraction limited beams e < l/4p
- Partial lasing
- Why is energy recovery needed:
    - 1.3 GHz pulses --- 77 pC --- 5 GeV ➔ 500 MW power (ERL design)
    - 120 Hz pulses --- 1nC --- 15 GeV ➔ 1.8 KW power (LCLS)
    - 1 MHz --- 1 nC --- 3 GeV ➔ 3 MW
- Gun design not yet available for full ERL/FEL operation

Photon sources and laser-based sources - Conventional lasers are the ultimate source for spectral ranges from IR to UV. They provide the highest powers in combination with complete control over the electromagnetic field amplitude and phase from cw to femto- or attoseconds. The extension of the laser principle towards the UV ends at ~150nm (commercial) and ~1…10nm (laboratory table-top x-ray lasers"), respectively. Physical barriers include active materials (ions), tunability, and pump power scaling. Nonlinear frequency conversion in the VUV generally rests on high intensities, provided by short-pulse driver lasers (e.g. High Harmonic Generation HHG in gases). Barriers are decreasing conversion efficiencies towards short wavelengths in combination with limited average power of the driver lasers. Special situations arise at relativistic intensities > 10^{18} W/cm^2, by interaction with relativistics electrons. Examples are sources based on inverse Compton scattering or plasma surface harmonics.

The characteristics of high harmonic generation: Attosecond VUV pulses are attosecond pulses, discrete (odd) harmonics, limited tunability, linear polarization and the conversion efficiency is 10^{-5} at 100 nm and less than 10^{-7} at 10 nm.

The EUV spectrum has attosecond pulses, discrete (odd) harmonics, limited tunability, linear polarization and the conversion efficiency is 10^{-5} at 100 nm and less than 10^{-7} at 10 nm.

Eberhardt showed a comparison of peak brilliance with accellerator-based sources.

In summary, with laser-based sources, Attosecond pulses:

- While considerable R&D is still required for these novel VUV- and X-ray sources, the dynamics of the field gives rise to high expectations for a "bright future
- While laser based sources in general are single user experiments, major resources (at the 10^8€ level) have been allocated to construct novel laser based VUV- and X-ray facilities or combinations of lasers and accelerators
- Open issues like stability, average power, broad band spectral coverage, lack of circular polarization etc. make a synergetic coexistence between laser- and accelerator-based VUV- and X-ray sources a foreseeable and fruitful future scenario
- Scientists should benefit across fields

Photon Source Properties and the correlation with science examines comparing magnetic materials and materials sciences with environmental sciences. There are X-ray needs, a high average brillance and tunability (spectromicroscopy).

Next, **Eberhardt** looked at Photoemission Microscopy: Imaging Catalytic Function - nm spatial resolution meets surface sensitivity and chemical specificity. He showed the difference between catalysis and environmental sciences.

The SMART project has design specifications of spatial resolution 2 nm and energy resolution 0.1 eV. It requires high average brilliance, energy resolution/tunability and space charge limitations.

In exploring the materials properties of size-selected clusters, XPS has high peak brilliance (pulsed source) and synchronization. (N)EXAFS, CMXD (ion trap) has high average brilliance and tunability.

The movies of chemical reactions involves analyzing and controlling photochemistry and photosynthesis. From XPS and scattering to high peak brilliance provides fs synchronization.

In summary, photon sources is a science for future generation X-ray sources, is very compelling, source parameters are needed and are not covered by a single type of source. There is high peak brilliance, Fs – synchronized pulses and full coherence. In addition, there is a high average brilliance, excellent energy resolution, ready tunability and many pulses. Lastly, you have attosecond synchronized pulses.

At 3:07 p.m., **Hemminger** began a discussion by asking Committee/Sub-Committee members to look at the report at how it exists today and how it can be improved.

Hemminger said we need high-level, instead of word-smithing comments. He said "if something is edited out, it can be put back in after discussion. We can discuss and transmit these via email." These edits should be sent to **Crabtree**.

Sylvia Ceyer said the report needs to address the hard core chemistry questions. "We can get broad information about photon stabilities. This is what we need in the future."

Martin Moskovits congratulated everyone who drafted the report. "Every section begins with an application. You can see the correlation. Most of this information will be very valuable. The one thing I did not see in the report was an outreach to the new population of users who discover these tools."

Hemminger agreed the new user outreach should be included. He also questioned if all user communities had been addressed.

Hemminger added "Let's think of the audience of this report. This is a different report that we have written recently. This should provide advice to those at BES. Can we use components of it? They have provided an opportunity to provide the next level of science drivers."

Kung said "it will help the Office of Science to formulate for the next 10 years. We should summarize it in a compelling way with a demonstration. The techniques have to there."

George Flynn asked for suggestions on how to do this, with the information summarized for us. He also questioned how many users would be needed for the machines to be beneficial.

Pedro Montano said 20% of the users. Most must go beyond the light sources.

Bruce Gates said "it seems the 'tone' is light source and there needs to be more. We need to have the requirements of characterization. The methodology should include characterization techniques. We need to recognize the future light source is more than just the light source."

Kate Kirby said she was having a hard time with the report. She questions if the current agenda can be transformed into new science. "The language is not consistent. It needs to parallel and more synergistic."

Crabtree said the Committe/Sub-Committee will work "in sync" to make sure both reports are "connected." He suggested having two reports, one being more high-level and technical. Both will be somewhat different.

Simon Bare said he agreed completely with **Kate Kirby's** comments.

William McCurdy Jr., said there have been workshops and gatherings to make a list of the numerous opportunities. In these reports, he believes it lacks "answering the questions." We need to make the connections between the nine areas and how X-rays affect each. The goal is to make clear that it is more than just light source, more complicated.

Nora Berrah agrees there needs to be more details.

Bare suggested "look at the charge of the report, when integrating the information in each and then expand on the information about photons."

Douglas Tobias said that "the organization of the report is key."

Bruce Kay said to identify the best science.

McCurdy Jr. said the core of the scientific case is to address questions. He cited an example that we have to make connections in order to explain things to other countries about the broad number of problems that need to be addressed.

Sylvia Ceyer said she agrees completely.

John Tranquada suggests revising certain statements to be more specific. He questioned if certain parts of the reports were "overstated."

Martin Moskovits said there are many techniques. Certain points have to be made with the specifics addressing questions that are being asked.

Bruce Gates said "we must wrap all of the different elements into the same experiment."

McCurdy Jr., added that we are not consistent in what we need to explain. "We need to acknowledge the experiments that can be done 10 years from now to a very large community."

George Flynn said he was confident that **Crabtree and Kastner** would do an excellent job splitting the reports into two separate documents.

Laura Green said this "is a very exciting report."

Kathleen Taylor thinks the report is very impressive and gets to the key issues. It is great to fulfill what is stated. She said she hopes that nothing is the report is overstated.

Hemminger asked **Crabtree** if he would provide a sypnosis tomorrow morning of everything we have discussed thus far. **Hemminger** said he has heard the report was fragmented instead of a book of wisdom. He heard it was written in more than one voice. The challenges need to be highlighted and strengthened. We should not concentrate solely on facility science. We need to integrate all sciences. This report should act as an advisory, showing more action of how we plan to get tasks accomplished. The report should include more visionary themes and topics.

The organization of the report needs to have an expanded executive summary, have an introduction and display vision and message of report. **Hemminger** believes this will be the part of the report that will most liely be read.

Hemminger is concerned over the past few years, we have been talking about what can get accomplished by doing the recommended tasks. He believes we need to concentrate on what will not be accomplished or can't be done if the recommended items are not addressed. We need to show examples. He said "we can't do X, without doing Y." This needs to be every prominent throughout the report.

McCurdy Jr., said "the document does not sit inside one department specifically."

Harriet Kung said it is highly desirable to have this report by April.

Gates said the report should state what we can do and why it is so important. "It needs to state the obvious."

Hemminger said "in the past, the Committee/Sub-Committees have had a 'homework assignment' to work out these issues. Several of our BESAC members have agreed to assist **George** and **Marc** with making incorporating the changes we have discussed this afternoon. **George** will provide an update tomorrow morning concerning implementing these changes."

At 4:28 p.m., **Hemminger** asked for public comment.

Rick Osgood, Columbia University, suggested incorporating the report should put an emphasis on scattering.

Murray Gibson, Argonne National Laboratory, said as a physicist, he agrees we should write about history, but need to put our focus on the future. He said imaging is important and has a great potential in the next 20 years in what could be the "imaging revolution."

Alan Hurd, Los Alamos National Laboratory, said in the next generation, photon scattering will see "explosive growth in the community." He added that it will be interesting to look at the data along with neutron scattering. The "pro-team" has started to grow in photons and neutrons. He requested BESAV look at this in the near future and urged authors to look at this with a global view.

Hemminger said he would start the meeting tomorrow morning with an hour set aside for the new science report and discuss what type of roll-out we should look at in getting this report distributed. "We need to advertise the report to keep pressure on the people appreciate the fundamentals of science."

With no additional public comment**, Hemminger** adjourned the meeting at 4:35 p.m.

Friday, February 27, 2009

At 8:32 a.m., **Hemminger** called the meeting to order. He said we would start the meeting off with a short discussion on the report the Committee discussed in November 2008. BESAC members should have a copy in advance to review. We must get the report in front as many people as possible

Hemminger introduced to **George Crabtree** to discuss the *New Science for a Secure and Sustainable Energy Issue*. Again, he and **Marc Kastner** served as Co-Chairs for the New Era Sub-Committee. **Crabtree** provided an outline of his presentation – discussing imported oil and carbon dioxide (main focus and captured many problems), breakthroughs for next generation sustainable energy, new science breakthroughs that are within reach (very important) and recommendations for the Sub-Committee.

Next, **Crabtree** discussed one of the major problems – the dependence on imported oil. "The gap between consumption and production will continue to be greatly different." During the 1970s, production peaked and has continued to decrease over the past few decades, while consumption (millions of barrels per day) has continued to increase greatly. The cost to the economy has been a staggering $700B per year in 2008, during the recent peak prices. Currently, it is costing $200B per year. We have transferred to foreign oil producers. Currently, we need to look at the unpredictability and the threat of interruption regarding the economy, lifestyle and national security. We must find alternatives to imported oil through biofuels, electricity and solar fuels.

Another problem is greenhouse gases and climate change. Approximately 66 percent of carbon dioxide emissions come from power plants and automobiles and have risen steadily over the past 50 years. There are also permanent changes in weather patterns, agricultural networks and coastal geography. The cost of accommodation is higher than preventative costs of reducing emissions.

In examining oil and carbon dioxide, it is "woven into our fabric" that we drive our cars on imported oil, with unfettered emissions of CO_2. Alternatives require fundamental changes in business as usual. We must find more sustainable, next generation, energy technology.

In sustainable next-generation energy technologies, solar electricity is a fully sustainable energy chain. It last a long time, does no harm to the environment and leaves no change. "The scientific breakthroughs needed are lower costs, higher efficiency photovoltaics, third generation materials and nanostructures, as well as electricity storage," **Crabtree** said.

In carbon sequestration, the sustainability profile lasts a long time, which is not good or bad news regarding emissions, does no harm and leaving no change in sequestration is not good news. Unfortunately, it depletes coal resources for hundreds of years, allows carbon dioxide into the environment and the effect can last a thousand years. The breakthroughs needed are chemical reactivity with rocks in extreme environments, migration through porous rocks, geologic monitoring and predictive modeling, as well as leakage routes to the atmosphere. Although we have hundreds of years of supply, we will eventually reach limits. It is not renewable like sunlight and so gets only an average score. Sequestration gets a high sustainability score for not emitting carbon dioxide, but a "wait and see" score for underground storage. There are many unanswered science questions – we do not know how harmful it might be. Sequestration leaves many changes – coal is removed from the earth, carbon dioxide is injected into the earth.

With nuclear electricity, it depletes uranium resources for hundreds of year and nuclear wastes must be stored. The breakthroughs needed are materials for extreme environments high temperature, high radiation flux, high corrosivity as well as geologic monitoring and modeling. Similar tradeoff to sequestration: carbon dioxide in the atmosphere is traded for radioactive waste underground.

In replacing conventional oil, biofuel lasts a long time, does no harm and leaves no change. Oil sands and shale and (coal to liquid) place 50 percent more carbon dioxide in the environment. The breakthroughs needed are cellulosic breakdown to sugar or fuel, as well as chemistry of oils sands and shale to fuel.

In electricity transportation, the sustainability profile lasts a long time, does no harm and leaves no change. The electric motor is typically more than 90% efficient, compared to 25%-30% for gasoline engines. "It is much simpler, with one shaft moving inside wire coils," said Crabtree. "The gasoline engine has valves, fuel injectors, and high temperature explosions several times per revolution and exhaust gases. Two ways to supply electricity are from a battery and ultimately the grid, as well as from a fuel cell with local supply of hydrogen. More energy in hydrogen with fuel cell, batteries are a major weak link in the electric vehicle energy chain. The sustainability profile depends entirely on production method – the electric car itself is fully sustainable. The breakthroughs needed are more than 2-5 times higher energy density in batteries as well as catalysts, membranes and electrodes in fuel cells.

In looking at the grid in sustainable energy enabling technology, the demand is higher in the eastern part of the U.S. Wind and sun occur more frequently in the western part of the U.S. The breakthroughs needed are long distance reliable and efficient delivery of electricity.

In storing energy, there are two options – to store intermittent solar and wind electricity and electrify transportation with plug-in hybrids and electric cars. Batteries have 30-50 times less energy density than gasoline. Beyond batteries, chemical storage and fuel cells equal electricity. The breakthroughs needed are two-five times increase in battery energy density and 10-20 times increase through chemical storage and fuel cells.

In examining traditional energy versus sustainable energy, traditional energy has commodity materials and disposal fuels, combustion, heat that leads to useful work. Sustainable energy requires controlling complex, functional, high-tech materials and chemistry, which is very different from traditional energy. It includes the use of sunlight, wind, water and geothermal biomass, direct conversion (high-tech materials and chemistry, such as photovoltaics, electrodes, superconductors and catalysts), electricity biofuels for useful work.

"We are now at the dawn of a new era," said **Crabtree**. "We are able to build materials with atom-by-atom precision, predict behavior of materials that have not been made and design materials for specific tasks. The breakthroughs to next generation sustainable energy technologies are now within reach."

There are challenges and opportunities that lie ahead. We must begin "weaning" ourselves from imported oil and carbon dioxide emission, which require structural change, not a refinement of business as usual. Next-generation sustainable energy technologies must operate at far higher performance, with far more complex, functional, high-tech materials. Developing these materials require scientific breakthroughs, which means we must control materials performance and chemical change at atomic, molecular lengths scales and sub-femtosecond time scales. Lastly, scientific breakthroughs in materials and chemical change are key. We must replace the economic drain of imported oil with economic growth from exporting next-generation energy technologies. The next generation energy technologies will be born. "Will we be buying or selling these new technologies? **Crabtree** asked. "We want to be sellers."

Since 2002 the BESAC and BES workshops have identified the roadblocks to next generation sustainable energy technologies. "We know what they are," **Crabtree** said. "The challenge now is to overcome them. Each one of these reports generated from the workshops is a treasure trove of information. They are long, 150 or more pages of good, well-thought information. If you want a quick overview, read the executive summary, the introduction and the conclusions. They are short; you can read them in an hour for each report."

Crabtree closed his presentation by offering the following recommendations:

- "Dream Teams" of the best scientists working with the best tools and focused on the most important problems are needed to achieve breakthroughs and transformational change (take the best from around the country and have them work together)
- The BES Energy Frontier Research Centers will launch these teams: an essential first step
- BES must launch an aggressive program to recruit and train the best and the brightest students and early career scientists (problems that are decades long. We need energy scientists and new talent right away).
- A massive and sustained investment in BES is needed immediately to achieve the breakthroughs in materials and chemical change needed for next-generation energy technologies (this needs to start immediately)

"The problems are so difficult that they cannot be solved by single scientists working alone," said **Crabtree**. "The best scientists will not usually be located at a single institution – they must be drawn from across the country. EFRCs are a model for launching "Dream Teams," but this is only testing the water. We need to refine and enlarge the concept, until it has the critical mass and the momentum to actually solve the basic science roadblocks to next generation sustainable energy technologies."

Hemminger asked the Committee/Sub-Committee for comments. He said he appreciates **George** and **Marc's** hard work.

Bruce Gates said he was enthusiastic, but needs to see more evidence when using phrases like "fundamental research needed now. We haven't made the case. You have asserted that we need the funding, but the evidence needs to be stated clearer."

Crabtree said we do not want to have an "open hole" and that a few more drafts may be needed.

Marc Kastner said "When we made our presentation in Washington, the investment is a massive issue."

Hemminger said this is going to continue to evolve, but agrees that there needs to be specific examples. He said "**George** provided superconductivity examples, and the breakthroughs that are needed. But, we need to explain why we need to do something different and provide more and better examples."

Bruce Gates added "We have to explain how science works."

Bruce Kay suggested "expanding on the information in the boxes."

Crabtree said "It will depend on the audience. You do not want to get too technical."

Bruce Gates said to "include scientific methods."

Laura Green said "With superconductors, if we had more comfortable funding and are more competitive with other countries, she believes there would be more excitement."

Hemminger said the one question in **Crabtree's** presentation that should stand out the most is "Are we going to be buying or selling?"

At 9:17 a.m., **Hemminger** requested **Marc Kastner** provide an outreach to new science."

With the outreach for the *New Science* report, **Kastner** said the Sub-committee created a one-page summary and made an effort to get the report read by as many opinion- and decision-makers as possible. He said the New Era Sub-committee held a conference call to decide on the list of people who we wanted to get they wanted the report sent to read. Just a few of the organizations included APS, ACS, NRC/NAS/NAE, others in Germany, Japan, Belgium, among others. In addition, the report was sent to Senators Bingaman, Finestein, several Representatives and opinion makers, such as former Lockheed Martin Chairman and CEO Norman R. Augustine, Tom Friedman and university presidents. **Kastner** stated that he had received a lot of help from the MIT and the University of California.

He said MIT Geophysics Professor and Head of MIT's Earth, Atmospheric and Planetary Sciences Department Maria Zuber attended an Innovation Roundtable on December 15, 2008 and discussed the importance of science. She was very excited at the roundtable and was invited by Speaker Nancy Pelosi and Congressman Rush Holt. Zuber was chosen by Speaker Pelosi to testify at the House Democratic Steering and Policy Committee Hearing January 7, 2009. Zuber specifically mentioned and passed out copies of the BESAC report and urged funding for EFRCs.

The following is the testimony from Zuber that appeared on the MIT Web site:

"Funding for research and education in science and technology should be a major priority in the economic recovery package Congress will soon be talking up," said MIT geophysics professor Maria T. Zuber in testimony she gave on Jan. 7 before the Steering and Policy Committee of the U.S. House of Representatives.

"Energy and climate could be our Sputnik challenge -- a new way to infuse our best talent into our science and technology system," said Zuber. The launching of Sputnik by the Soviet Union in 1957 spurred major U.S. investment in education in science, math and technology and led to a boom in those areas.

Zuber emphasized that while direct economic stimulus plans could lead to short-term economic benefits, it takes education and technological innovation to create lasting, long-term economic growth and job creation.

"We need to bolster existing high-growth innovation areas and we will need to create new areas," she said. "One path ahead is clear: the country is on the cusp of a revolution in energy science and technology." With the energy sector already at $2 trillion in the U.S. economy, "we don't have to invent a new market; we have to find new ways to grow and dominate an existing but nascent market." Such investments will "not only create jobs, it will also have positive effects on the environment, and on the nation's technological leadership in the world," she said.

Toward that end, she suggested, the DOE could fund many more of the 270 applications it already received for the creation of EFRCs, many of which were very highly rated but were not accepted because of limited funding. In addition, major upgrades to the nation's electric grid are needed in order to enable greater efficiency and wider use of renewable energy.

Citing a recent DOE report, Zuber said "we must develop the breakthrough energy technologies that will free us of our dependence on foreign oil, reduce our carbon emissions and create economic growth, but that will only happen with immediate, real investments."

But energy cannot be the whole story, Zuber said. It is a so essential to increase the funding for research in a wide variety of areas, including health, aerospace, and basic science. Toward that end, supporting the purchase of major research instrumentation for colleges and universities could produce a stimulus for research while helping to train the scientists and engineers of the future. In addition, support for students in the form of fellowships to sustain important research will help to prepare a new generation of technicians and scientists.

Direct investment in education by supporting the best teachers is another key area needed to bring about long-term growth in the nation's technology base, Zuber said. "Investment in highly qualified teachers who inspire, encourage and challenge students" is crucial, she said.

Zuber, who is the E.A. Griswold Professor of Geophysics, was invited to testify by House Speaker Nancy Pelosi. Also on the panel were economists Mark M. Zandi and Martin Feldstein, former Secretary of Labor Robert Reich.

Hemminger, Crabtree and **Kastner** also briefed House and Senate staffers on February 3, 2009 (important Committees were represented); the following day, briefed the Center for Strategic and International Studies (CSIS) (big audience of 150 people); and Crabtree would testify for Bingaman committee.

The CSIS meeting stated "The pathway to a secure, low-carbon energy economy will undoubtedly require accelerated development of a suite of advanced technologies, underpinned by a sustained commitment to research and development. Many options hold great promise – solar photovoltaics, efficiency, battery and storage technologies – but their realization will rely on further advances in our understanding of basic science."

Crabtree said The House convinced the Senate to add money to the Office of Science.

Hemminger asked the Committee/Sub-Committee for comments.

Kate Kirby congratulated **Kastner** on the success. She believes it captures the essence of science and gets people excited. "The Committee has done a fabulous job to get to the Government and Congress." She added that if universities see the future, the available funding will be tremendously valuable for future research."

Nora Berrah said it is a "wonderful document." She suggested that all Committee members become more active and involved in getting the message out.

Simon Bare said he could "assist with specific organizations and would be glad to assist **George**."

Bruce Gates said he was concerned the report would lose its "timeliness" if we do not get the message out as soon as possible.

Hemminger said "universities are good, but people who run universities are not scientists. We must make sure the report is getting into the right hands."

Once again, **Hemminger** said one of the messages around the stimulus bill was whether we would be buyers or sellers. **Hemminger** congratulated **George** for incorporating that slide and believed it to be very effective.

At 9:30 a.m., **Hemminger** declared a break.

At 9:50 a.m., **Crabtree** presented comments from yesterday's meeting.

Crabtree said he appreciated all of the Committee and Sub-Committee members that worked with him and **Kastner** in the night before to incorporate new ideas into Photon Workshop Report.

Some of the comments included:

- Making a better connection between the New Era report and energy
- Integrated wisdom
- Visionary outlook
- Make the report have a single voice and style
- Beyond the source photons – integration of other characterization methods; supporting capability (e.g., for catalysis); theory; computation; data manipulation; endstations, optics, detectors; and dream teams
- Science communities beyond materials and chemistry (e.g., life, earth and environmental)
- Train next generation of scientists

- Add more sidebars relating to macromolecular crystallography (example of new communities); replicate photosynthesis by studying photosynthesis (energy); dynamics of life sciences; successes for industry

Additional comments and the "elevator messages" included:

- Controlling matter and energy in complex materials creates a tipping point for sustainable energy
- Observing phenomena on relevant length and time scales is beyond reach today (Observe → Understand → Control)
- Needs
    - Temporal evolution of electrons, spins, atoms, and chemical reactions, down to fs
    - Probing isolated nano-objects or nano-regions of inhomogeneous samples, by spectroscopy with an energy resolution smaller than the intrinsic line width, or by imaging with a spatial resolution at the atomic limit
- Today's photons fall short
    - Peak brightness for temporal resolution and dynamics (fs/attosec resolution)
    - Average brightness for spatial resolution (nm imaging of isolated objects)
    - Coherence for lenseless imaging, holography
- Photons are not enough, we need the source, optics, end-station and detector, as well as theory and experiment (including in situ synthesis and real-time observation)
- Tools of control science profit broader communities as well life science, earth science, environmental science
- Dream teams, workforce development

Crabtree said that the goal of the Sub-Committee would be to provide a more uniform style. The goal is to improve the report to make it more comprehendible for all audiences. The executive summary and introduction would be written to have a more "visionary" feel and needs to be more exciting and provide more background information. This section has been assigned to **John Sarrao. Michael Norman**, will bring more clarification to Chapter 6 with support from Chapter 4 concerning photon science drivers. The grand themes of photon science will be written by **Crabtree** and **Sarrao**, with cross-cutting challenges from Chapter 3. After incorporating all of these comments, the conclusion will be re-written by **Crabtree**.

With that in mind, the second draft of the report will have a refined structure to include:
Section 1 - Executive Summary

Section 2 - Background
Section 3 - Cross-Cutting Challenges
Section 4 - New Scientific Opportunities
Section 5 - Photon Sources
Section 6 - Conclusions
Appendix 1: Related Studies.
Appendix 2: Photon Attributes for Individual Scientific Opportunities

Crabtree concluded by stating "we are taking the pieces we have already written and making minor edits, changing the order slightly and expend on certain messages, using the standard Basic Research Needs format. **Franz** and **Wolfgang** will give this revision to a new writer and the report will have a fresh look for those who are not topic experts."

At 10:05 a.m., **Hemminger** thanked **Crabtree, Kastner** and all of the Committee and Sub-Committee members that had volunteered and "stepped up to the challenge and assisted in making this report the best it can be." He asked if there were additional comments regarding the revision.

Sylvia Ceyer said in the introduction, we need to address problems and state how this type of science impacts how and what we want to study.

Douglas Tobias said the report looks good, but questioned if there will be something in the introduction regarding photon science drivers.

Crabtree said "yes, everything will be addressed in the introduction, including the cross-cutting challenges."

Bruce Kay suggested that a few paragraphs of where we are today (the current status) and a reflection on how far we have come (the past).

Crabtree agreed and said that would be included in the "elevator messages."

Bruce Kay added that having a "dream team" is not a new idea and that has always been a goal with every workshop and report.

Crabtree agreed, but said it is getting more important for the best (most educated and scientifically inclined) to work together.

Hemminger said "Five years ago, there was opposition to a 'dream team' and having a single investigator. The study should be emphasized and a mechanism that is embraced within the scientific community."

Gates asked if there will be a "shorter, more condensed version of the elevator message."

Crabtree said that is "a great idea."

Hemminger asked if this should be a short one pager or a glossy five page version.

Gates said it could have a significant impact. "We should know who our audience is we are trying to target in advance."

Hemminger questioned how many of the specific audiences will be willing to read the report. We need to tell Harriet, BES and the Office of Science on what we think of the topic in one report and have another report that is not as specific.

Nora Berrah told **Crabtree** he had done a great job and congratulated him on the new outline and incorporating the changes. She said also liked the organization and thanked him, **Kastner** and the Sub-Committee for everything they had done.

Hemminger agreed with **Berrah's** comments and said it had taken a lot of dedication and hard work to get the revisions completed and once again thanked **Crabtree** and **Kastner** for their hard work in getting the revisions completed.

Hemminger also said "what we have done in previous reports is to identify the people who will implement the changes, make the modifications, then complete the BESAC report and get it out to the people who need to see it." We have had volunteers, such as **Michael Klein**, to look at the final version. The Committee anoints **George** and **Marc** to make revisions.

William McCurdy Jr., questioned the timescale of the project. He asked **Kung** if there was a date when she would like to see the report completed.

Kung said she would recommend receiving it by mid-April. "In six weeks, I would like to have the final 'glossy' copy that would convey our future planning."

Crabtree said that was "do-able."

Hemminger asked for a show of hands from the Committee/Sub-Committee for a show of hands to move forward with the report. All Committee/Sub-Committee members, with the exception of Simon Bare, approved.

Hemminger said the report should be distributed to universities and PowerPoint presentations could possibly be developed to "get the message out." He added that some of the reports would need to be more technical than others.

Gates said "We need to keep track of who has requested and asked for specific information."

Hemminger opened the floor to public discussion.

Hemminger said he would welcome concrete suggestions, PowerPoint slides and other information to incorporate into the report. "I know there are some good ideas and great examples out there."

There being no other public input, **Hemminger** adjourned the meeting at 10:29 a.m.

Respectfully submitted,
Raymond P. Johnson Jr.
March 19, 2009